Supplemental information:

Native electrospray mass spectrometry reveals the nature and stoichiometry of pigments in the FMO photosynthetic antenna protein

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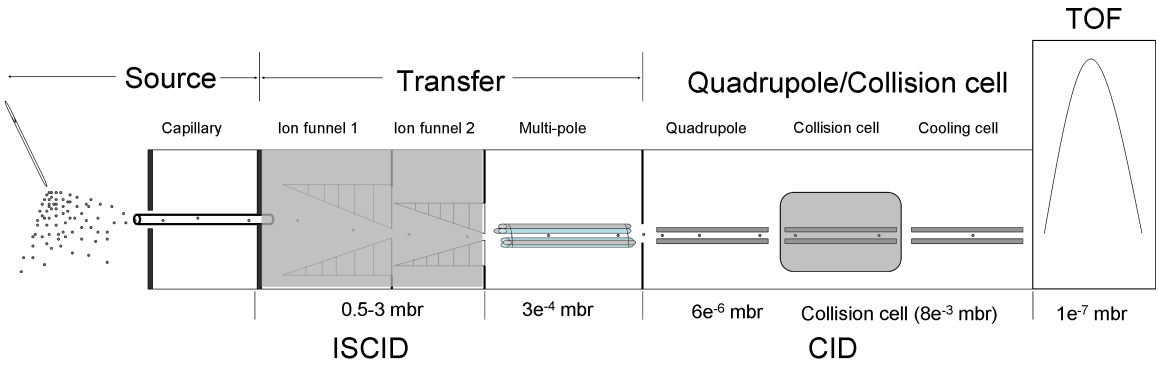
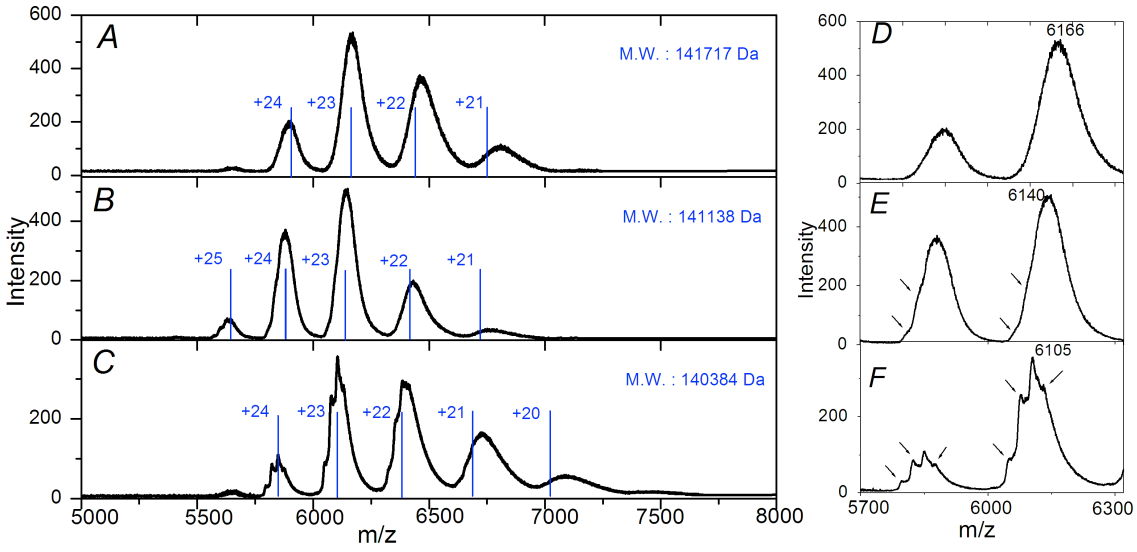
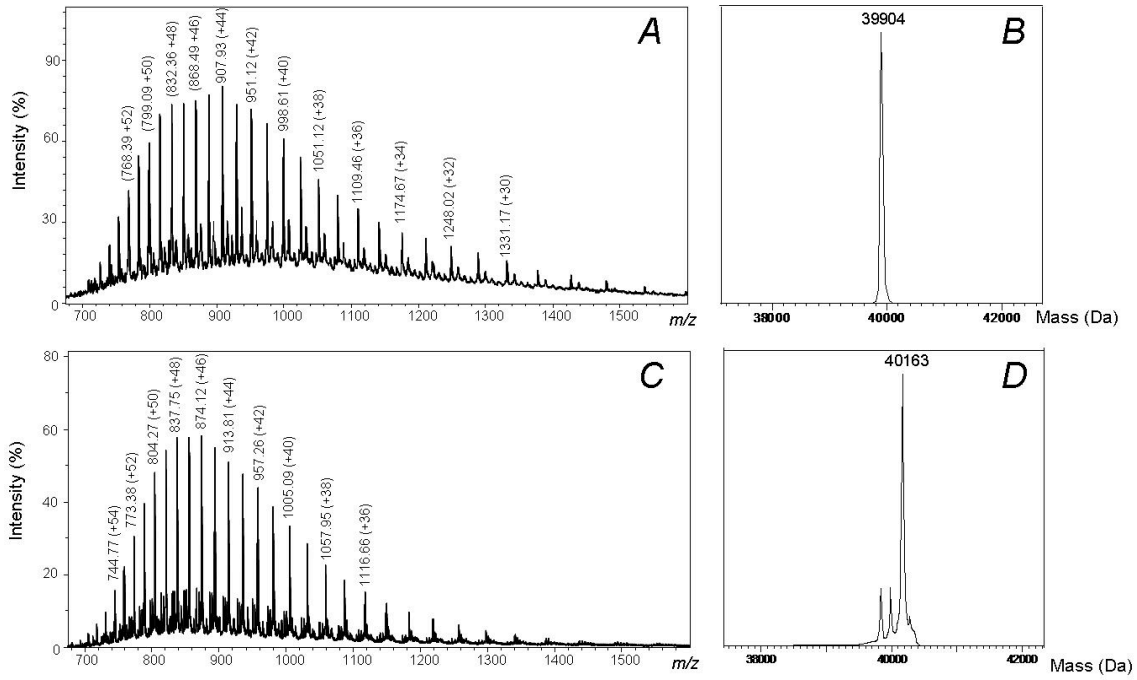


SI-Figure 1. Schematic picture of the ion source, ion transfer and mass analyzer in the Maxis Q-TOF instrument. Ions generated by nano-electrospray in the source pass through the capillary and are transferred through two ion funnels and a multi-pole. Ions are analyzed and selected in the quadrupole region and finally hit the TOF mass analyzer. The pressure at different regions are labeled, and collision induced dissociation (CID) could be performed at either the source region between the capillary and the ion funnels (ISCID) or in the collision cell at the quadrupole region.



SI-Figure 2. Mass spectra of intact AFMO complex by native electrospray and the charge-state simulations using the listed molecular weight (M. W.) with the base peak carrying +23 charges. Nano-ESI conditions: *(A)* voltage of ISCID: 30 V; CID: 10 eV *(B)* voltage of ISCID: 50 V; CID: 10 eV *(C)* voltage of ISCID: 150 V; CID: 10 eV. The vertical blue lines are theoretical *m/z* values for charge states +20 to +24 generated using the labeled MW; the +23 charge state was assigned to the base peak. *(D)-(F)* are the expansion of the +22 and +23 charge states in panels *(A)-(C)* with arrows indicating the appearance of shoulders. The shift of the labeled *m/z* indicates better desolvation of the complex.



SI-Figure 3. Mass spectra of denatured AFMO *(A)* and TFMO *(C)*, and their deconvoluted molecular weight *(B)* and *(D)*, respectively. The deconvoluted molecular weight of the AFMO protein matches that deduced from the protein sequence without the N-terminal MetAlaLeuPhe residues (theoretical molecular weight: 39,904 Da). The deconvoluted molecular weight of the TFMO corresponds to the value deduced from the protein sequence without the N-terminal Met. The two shoulders on the low mass side *(D)* correspond to the protein sequence without the N-terminal MetAlaLeu (39,979 Da) and MetAlaLeuPhe (39,831 Da) residues, respectively.